

Nonlinear Oscillator Hamiltonian from Nonlinear Differential Equation and Calculation of Accurate Energy Levels

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A new method for generating analytical expression of quantum Hamiltonian from non-linear differential equation with stationary energy level has been formulated. Further calculation of energy levels have been carried out analytically using and numerically using matrix diagonalisation method.

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Key words- Non-linear differential equation; energy level; matrix diagonalisation method, Perturbation theory, Non-linear oscillator.

I. Introduction

In classical as well as quantum mechanics there are a only few problems which can be solved exactly. It has been seen that many approximation methods have been applied to Harmonic oscillator with a view to bring new methods to limelight. However, to the best of our knowledge none of the published work [1-7] deals with the generation of quantum Hamiltonian from non-linear differential equation.

In this communication, we present an innovative method to derive quantum Hamiltonian from non-linear differential equation

II. Method

In one dimension differential equation can be written as

$$x'' + f(x) + F(x, x) = 0 \quad (1)$$

where $f(x)$ is a function of x and $F(x, x)$ is a function of x and it's derivative with respect to time. The form of $f(x)$ and $F(x, x)$ can be considered as

$$f(x) = \sum_l \alpha_l x^l \quad (2)$$

and

$$F(x, x) = \sum_{k,m} \lambda_{k,m} (x')^k x^m \quad (3)$$

The equation of motion can be written as

$$\frac{dx'}{dt} = -f(x) - F(x, x) \quad (4)$$

Now using the relation

$$\frac{dx'}{dt} = -\frac{dV(x)}{dx} \quad (5)$$

and

$$H = \frac{p^2}{2} + V(x) \quad (6)$$

we can get $V(x)$ as

$$V(x) = \int [f(x) + F(x, x)] dx$$

In the above H is considered as the Hamiltonian of the system in which $V(x)$ is the potential (potential energy) . Now we can write the Hamiltonian as

$$H = \frac{p^2}{2} + \int [f(x) + F(x, x)] dx \quad (7)$$

In order to simplify the form of H , we use the formalism of second quantization and express x and p in terms of creation operator, a^+ and anihilation operator, a as

$$x = \frac{1}{\sqrt{2w}} [a + a^+] \quad (8)$$

and

$$p = i\sqrt{\frac{w}{2}} [a^+ - a] \quad (9)$$

Using equations (8) and (9), we can write Eqn. (7) as

$$H = \frac{p^2}{2} + \frac{1}{\sqrt{2}w} \int [f(x) + F(x, x)](da + da^+) \quad (10)$$

III. Hamiltonian in Second Quantization form In the Eq(10) one has to use different forms of $f(x)$ and F to get the Hamiltonian in second quantization form.

III.A.Linear $f(x)$

Considering $f(x) = w^2x$ and $F(x, x) = \lambda(x)^2x$, the Hamiltonian in Eqn. (10) can be written as

$$H = [2a^+a + 1]\frac{w}{2} + \frac{\lambda}{16} + \frac{\lambda}{16}[2(a^+)^2a^2 + 4a^+a] - \frac{\lambda}{16}[(a^+)^4 + a^4] \quad (12)$$

III.B.Non-Linear $f(x)$

We also consider $f(x) = w^2x + \lambda x^3$ and $F(x, x) = \lambda(x)^2x$ and using Eqn. (10), the Hamiltonian (with $w = 1$) can be written as

$$H(1) = \frac{[2a^+a + 1]}{2} + \frac{\lambda}{4} + \frac{\lambda}{2}[(a^+)^2a^2 + 2a^+a] + \frac{\lambda}{8}[2(a^+)^3a + 2a^+a^3 + 3a^2 + 3(a^+)^2] \quad (13)$$

IV. Perturbation Theory In this section, we use perturbation theory to calculate the energy levels up to second order. The Hamiltonian can be written in terms of perturbed and unperturbed Hamiltonian as

$$H = H'_0 + H'_1 \quad (14)$$

where

$$H'_0 = [2a^+a + 1]\frac{w}{2} + \frac{\lambda}{16} + \frac{\lambda}{16}[2(a^+)^2a^2 + 4a^+a] \quad (15)$$

and

$$H'_1 = -\frac{\lambda}{16}[(a^+)^4 + a^4] \quad (16)$$

Using standard perturbation theory[6,7], the expression for ground state energy up to second order (considering $w = 1$) is

$$E_0 = E_0^{(0)} + E_0^{(1)} + E_0^{(2)} + \dots \quad (17)$$

where

$$E_0^{(0)} = \frac{1}{2} + \frac{\lambda}{16} \quad (18)$$

$$E_0^{(1)} = 0 \quad (19)$$

$$E_0^{(2)} = -\frac{3\lambda^2}{32(4 + 2.5\lambda)} \quad (20)$$

In Table-1 we present groundstate and first excited state energy of the Hamiltonian in Eq(14) for $\lambda = 0.1$. Further if one considers the Hamiltonian of the form

$$H = \frac{p^2}{2} + \int [w^2 x + \lambda x^3 + F(x, x)] dx \quad (21)$$

In this case with $w = 1$ we get

$$H(1) = H'_0 + H'_1$$

where

$$H'_0 = \frac{[2a^+a + 1]}{2} + \frac{\lambda}{4} + \frac{\lambda}{2}[(a^+)^2 a^2 + 2a^+a] \quad (22)$$

and

$$H'_1 = \frac{\lambda}{8}[2(a^+)^3 a + 2a^+ a^3 + 3a^2 + 3(a^+)^2] \quad (23)$$

In Table-1 we present groundstate and first excited state energy of the Hamiltonian in Eq(14) for $\lambda = 0.1$.

V. Matrix Diagonalization Method (MDM)

In order to get accurate energy levels of this Hamiltonian (Eqn. (10)) we use matrix diagonalisation method as follows. Now we solve the eigen-value relation [8-10]

$$H\psi = E\psi \quad (24)$$

where

$$\psi = A_m |m\rangle_w \quad (25)$$

For Hamiltonian in Eqn. (12),

$$H = [2a^+a + 1]\frac{w}{2} + \frac{\lambda}{16} + \frac{\lambda}{16}[2(a^+)^2a^2 + 4a^+a] - \frac{\lambda}{16}[(a^+)^4 + a^4]$$

we obtain a three term recurrence relation [as

$$A_{m+4}P_m + A_mR_m + A_{m-4}T_m = 0 \quad (26)$$

where

$$P_m = \langle m|H|m+4 \rangle_w \quad (27)$$

$$R_m = \langle m|H - E|m \rangle_w \quad (28)$$

$$T_m = \langle m|H|m-4 \rangle_w \quad (29)$$

Here $|m \rangle_w$ is the m th state wave function of Harmonic oscillator with parameter w . On solving the three term recurrence relation using matrix diagonalisation method, we calculated first five energy levels for the Hamiltonian given in Eqn. (12) and reflected the same in Table 1.

The Hamiltonian in Eqn. (13)(with $w = 1$) can be written as

$$H(1) = \frac{[2a^+a + 1]}{2} + \frac{\lambda}{4} + \frac{\lambda}{2}[(a^+)^2a^2 + 2a^+a] + \frac{\lambda}{8}[2(a^+)^3a + 2a^+a^3 + 3a^2 + 3(a^+)^2]$$

In order to get the accurate energy eigen-values of this Hamiltonian, we use matrix diagonalisation method as stated above. In this case, we obtain a three term recurrence relation as

$$A_{m+2}Q_m + A_mR_m + A_{m-2}S_m = 0 \quad (30)$$

where

$$Q_m = \langle m|H(1)|m+2 \rangle_w \quad (31)$$

$$R_m = \langle m|H(1) - E|m \rangle_w \quad (32)$$

$$S_m = \langle m|H(1)|m-2 \rangle_w \quad (33)$$

VI. Results and Conclusion

In the present paper, we accurately calculate the numerical values of energy levels of the Hamiltonian obtained from non-linear differential equation using matrix diagonalisation method. Further we noticed that the numerical value of the ground state energies for the above two Hamiltonians nicely matches with the analytical value. For example: the ground state energies of Hamiltonian (Eqn.(6)) in the present method is found to be 0.506 029 which matches nicely with the previously reported analytical value (0.506 03). Similarly, for the Hamiltonian in Eqn. (13), the present convergent value for the ground state is 0.523 76 whereas the previously reported analytical value is 0.523 77. In our formalism, we practically developed a new method for generating Hamiltonian from any non-linear differential equation of second order. Further one can calculate its energy levels either numerically or analytically.

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Table -I

First two energy levels of the Hamiltonian Eq(12) and Eq(13)

n	$E_n^{(0)}$	$E_n^{(1)}$	$E_n^{(2)}$	E_n	Hamiltonian
0	0.506 25	0	-0.000 220	0.506 03	Eq(12)
1	1.531 25	0	-0.001 077	1.530 173	
0	0.525	0	-0.001 222	0.523 778	Eq(13)
1	1.625	0	-0.009 375	1.615 625	

Table -II

First five energy levels of the Hamiltonian (Eq(12))

n	Size(9x9)	Size(19x19)	Size(29x29)	Size(39x39)
0	0.506 029 039	0.506 029 038	0.506 029 038	0.506 029 038
1	1.530 172 680	1.530 169 441	1.530 169 441	1.530 169 441
2	2.578 092 128	2.578 076 954	2.578 076 954	2.578 076 954
3	3.649 049 855	3.648 997 679	3.648 997 673	3.648 997 673
4	4.742 400 314	4.742 253 427	4.742 253 401	4.742 253 401

Table -III

First five energy levels of the Hamiltonian (Eq(13))

n	Size(9x9)	Size(19x19)	Size(29x29)	Size(39x39)
0	0.523 767 849	0.523 767 849	0.523 767 849	0.523 767 849
1	1.615 478 755	1.615 478 611	1.615 478 611	1.615 478 611
2	2.791 344 321	2.791 342 192	2.791 342 192	2.791 342 192
3	4.044 414 426	4.044 094 127	4.044 094 126	4.044 094 126
4	5.369 741 578	5.368 297 477	5.368 297 470	5.368 297 469